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Maximally resonant polygonal systems☆

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ABSTRACT

A benzenoid system G is k-resonant if any set F of no more than k disjoint hexagons is a resonant pattern, i.e, $G - F$ has a perfect matching. In 1990's M. Zheng constructed the 3-resonant benzenoid systems and showed that they are maximally resonant, that is, they are k-resonant for all $k \geq 1$. Recently, the equivalence of 3-resonance and maximal resonance has been shown to be valid also for coronoid systems, carbon nanotubes, polyhexes in tori and Klein bottles, and fullerene graphs. So our main problem is to investigate the extent of graphs possessing this interesting property. In this paper, by replacing the above hexagons with even faces, we define k-resonance of graphs in surfaces, possibly with boundary, in a unified way. Some exceptions exist. For plane polygonal systems tessellated with polygons of even size at least six such that all inner vertices have the same degree three and the others have degree two or three, we show that such 3-resonant polygonal systems are indeed maximally resonant. They can be constructed by gluing and lapping operations on three types of basic graphs.

1. Introduction

Resonance is related to an aromatic sextet [2] in Clar's aromatic sextet theory and Randić's conjugated circuit model [7–12] and was first investigated for benzenoid systems [4,24,25]. Benzenoid systems are finite 2-connected plane graphs with every interior face bounded by a regular hexagon. A coronoid system is a benzenoid system with "holes" (non-hexagonal interior faces). A benzenoid or coronoid system is called *k-resonant* ($k \geqslant 1$) if any i ($0 \leqslant i \leqslant k$) disjoint hexagons of it are mutually resonant.

The 1-resonant benzenoid systems have been completely characterized [17]. The problem of constructing 2-resonant benzenoid systems has been not solved yet. However, 3-resonant benzenoid systems were constructed by Zheng [25] as follows.

Theorem 1.1 ([25]). *A benzenoid system is 3-resonant if and only if it can be constructed from a set of k benzenoid systems of the following four kinds by $k - 1$ fusing operations such that in each operation the glued edges are the edges marked only.*

Further, Zheng [24] showed that a 3-resonant benzenoid system is necessarily k-resonant for any $k \geq 1$. The concept of k-resonance was extended naturally to other polyhex graphs on planes, cylinders, tori and Klein bottles, as well as fullerenes on spheres. 3-resonant coronoid systems [1], toroidal polyhexes [13,21], Klein-bottle polyhexes [5,14], open-ended nanotubes [18], and fullerenes [16] are all k-resonant for any $k \geq 1$. So our main problem is to investigate the extent of graphs possessing this interesting property. For more information on k-resonance, please see [3,6,19].

We first consider graphs on a surface. A closed *surface* is a connected and compact Hausdorff space which is locally homeomorphic to an open disc in the plane. A surface, possibly with boundary, is simply a closed surface with a number of

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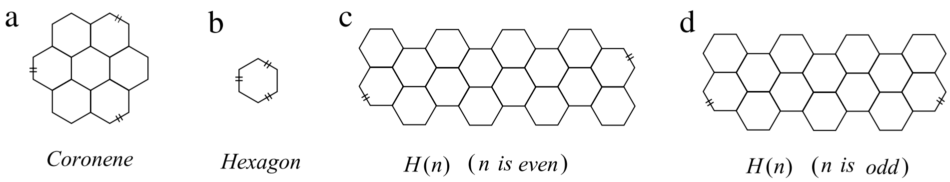

Fig. 1. Four kinds of benzenoid systems to construct all the 3-resonant benzenoid systems.

holes (open discs that have been removed). For example, the cylinder and the Möbius strip are orientable and non-orientable surfaces with boundary respectively. A graph G on a surface S is an embedding of a graph in S so that each face (a connected component of $S \setminus G$) is homeomorphic to an open disc in the plane, the boundary of each face is a cycle of the graph, and the boundary of each hole forms a subgraph of the graph.

We now define the k-resonance in a unified way as follows. For a graph G on a surface S, a set $\mathcal{H}$ of disjoint even faces of G is said to be a *resonant pattern* if G has a perfect matching M and the boundary of each face in $\mathcal{H}$ is an M-alternating cycle. If G has a perfect matching, an empty set is also a resonant pattern. A graph G on a surface S is called *k-resonant* $(k \geqslant 1)$ if any i $(0 \leqslant i \leqslant k)$ disjoint even faces form a *resonant pattern*. For plane benzenoid or coronoid systems, the exterior face and holes are excluded in resonant patterns. For fullerenes on a sphere, although pentagons may not be "holes", they are odd faces and thus are excluded. For open-end nanotubes, two ends are regarded as "holes".

For convenience, we propose a concept as follows. A graph G on a surface is called *maximally resonant* if any set of disjoint even faces of G is a resonant pattern, i.e., G is k-resonant for any $k \geq 1$. Hence the previous property becomes "3-resonance implies maximal resonance". Our problem is to study this property and characterize maximally resonant graphs on a surface. In addition to the above types of graphs, 3-resonant bipartite polyhedral graphs and boron–nitrogen fullerenes on spheres without holes are maximally resonant [15,20]. But two examples in the final part of this paper show that the property does not always hold.

In this paper we consider a plane polygonal system, where the infinite face is a natural "hole" and excluded from the resonant patterns. So, in the following, "face" in a plane graph always means a finite face (interior face). Let $\mathcal{G}$ be the class of 2-connected plane bipartite graphs such that each interior face is a polygon of even sides with size at least six and every inner vertex having degree 3 while the others have degree 2 or 3. In particular, $\mathcal{G}$ contains all the benzenoid systems.

The characterization for 1-resonant graphs G in $\mathcal{G}$ has been given in three equivalent ways: G is elementary (each edge is contained in a perfect matching) [22], G has a reducible face decompositions [22], and the boundary of G (the boundary of the infinite face of G) is resonant [23].

In this paper, we characterize all the maximally resonant graphs in $\mathcal{G}$. Like the benzenoid systems, we first obtain several "basic" kinds of 3-resonant graphs in $\mathcal{G}$, from which we then construct all the 3-resonant graphs in $\mathcal{G}$. To our surprise, the construction method for 3-resonant graphs in $\mathcal{G}$ is similar to 3-resonant benzenoid systems, although we ignore the geometrical features of the polygons. On the other hand, the polygonal systems constructed by our method are all maximally resonant, which implies that 3-resonant graphs in $\mathcal{G}$ are also maximally resonant.

2. 3-resonant graphs in $\mathcal{G}$ with no separating faces

The *inner dual* $D(G)$ of a plane graph G is the dual of G without the vertex corresponding to the infinite face of G. For any $G \in \mathcal{G}$, since each interior face of $D(G)$ corresponds to an inner vertex of G which has degree 3, $D(G)$ is a plane graph with each interior face bounded by a triangle. The number of 2-degree vertices is computed for graphs in $\mathcal{G}$.

Lemma 2.1. *Let $G \in \mathcal{G}$. Then G has at least six 2-degree vertices on its boundary.*

Proof. Let k_1, k_2 and k_3 be the number of 2-degree vertices, 3-degree vertices on the boundary and inner vertices of G, respectively. Suppose G has n vertices, m edges and f faces. Then

$$n = k_1 + k_2 + k_3$$

and

$$2m = 2k_1 + 3(k_2 + k_3) = 3n - k_1.$$

Since the size of the exterior face is $k_1 + k_2$,

$$\sum_{i \geqslant 6} if_i + k_1 + k_2 = 2m,$$

where f_i is the number of interior faces with size i in G. Then

$$n = \frac{2m + k_1}{3} = \frac{\sum_{i \geqslant 6} if_i + 2k_1 + k_2}{3}.$$

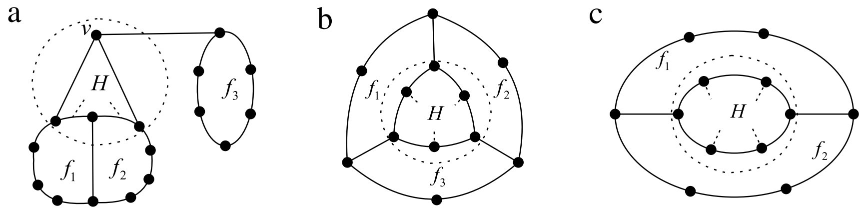

Fig. 2. Forbidden subgraphs of graphs in $\mathcal{G}$.

On the other hand,

$$f = \sum_{i\geqslant 6} f_i + 1.$$

Thus, for G, Euler's Formula $n - m + f = 2$ can be expressed as

$$\frac{\left(\sum_{i\geqslant 6} if_i + 2k_1 + k_2\right)}{3} - \frac{\left(\sum_{i\geqslant 6} if_i + k_1 + k_2\right)}{2} + \sum_{i\geqslant 6} f_i + 1 = 2,$$

that is,

$$6 + k_2 - k_1 = \sum_{i\geqslant 6} (6 - i) f_i \leqslant 0.$$

Since $k_2 \geqslant 0$, we have

$$k_1 \geqslant 6. \quad \square$$

Polygonal systems in $\mathcal{G}$ have all inner vertices with degree 3. Hence, the common boundary of two adjacent faces (polygons) consists of disjoint edges.

Corollary 2.2. *Let $G \in \mathcal{G}$. Then G has none of the following graphs as subgraphs:* (a) *two adjacent faces f_1 and f_2, which contain two neighbors of a vertex v, respectively, but do not contain v;* (b) *three pairwise adjacent faces that are connected by three disjoint edges; and* (c) *two faces sharing more than one edge (see Fig. 2).*

Proof. Suppose that G has one of these graphs as a subgraph. Then G contains a subgraph H (enclosed by the dashed cycle), which also belongs to $\mathcal{G}$ but has less than six 2-degree vertices on the boundary (see Fig. 2). That is a contradiction by Lemma 2.1. Hence, G contains no such subgraphs. $\square$

By Corollary 2.2, the following property is immediately obtained.

Corollary 2.3. *Let $G \in \mathcal{G}$. Then the common boundary of every pair of adjacent faces of G is an edge.*

Now we turn to the 3-resonant polygonal systems in $\mathcal{G}$.

Lemma 2.4. *Let $G \in \mathcal{G}$. If G has an inner vertex whose three neighbors are all inner vertices, then it is not* 3*-resonant.*

Proof. Let v be an inner vertex of G. Suppose that its three neighbors v_1, v_2 and v_3 are all inner vertices. Then there are three faces f_1, f_2 and f_3 of G such that $v_i \in V(f_i)$ and $v \notin V(f_1 \cup f_2 \cup f_3)$. By Corollary 2.2(a), f_1, f_2 and f_3 are pairwise disjoint. By the similar argument of Corollary 2.2, f_1, f_2 and f_3 are pairwise different. Then v is an isolated vertex of $G - f_1 - f_2 - f_3$. Hence G is not 3-resonant. $\square$

In the following, we first characterize 3-resonant polygonal systems without *separating faces*, where a separating face is one whose removal disconnects the graph. A face f of a plane graph is an *internal face* if all the vertices on the boundary of f are inner vertices.

Lemma 2.5. *Let G be a* 3*-resonant polygonal system in $\mathcal{G}$ without separating faces. If G has internal faces, then $D(G)$ is a wheel with odd vertices.*

Proof. Let f be an internal face of G and $f_1, f_2, \ldots, f_{2m}$ ($m > 2$) the neighboring faces of f in the cyclic order, each of which is adjacent to both the preceding face and the successor. Suppose that $f \cap f_i = e_i$ ($1 \leqslant i \leqslant 2m$). Then f_i and f_j are adjacent if and only if $i = j \pm 1$ or $\{i, j\} = \{1, 2m\}$ by Corollary 2.2(b). Let v_i ($1 \leqslant i \leqslant 2m - 1$) be the vertex of $V(f_i) \cap V(f_{i+1})$ not on f and v_{2m} the one of $V(f_{2m}) \cap V(f_1)$ not on f.

Suppose that there are other faces in G besides $f, f_1, f_2, \ldots, f_{2m}$. Then there is at least one, say f', containing some v_i, since G has no separating faces. Without loss of generality, suppose that v_1 lies on f'. Then v_1 is an inner vertex. Let v be the common end vertex of e_1 and e_2. Then v is an inner vertex whose three neighbors are all inner vertices. It is a contradiction by Lemma 2.4. Hence $f, f_1, f_2, \ldots, f_{2m}$ are the only interior faces of G and thus $D(G)$ is a wheel with odd vertices (see Fig. 3). $\square$

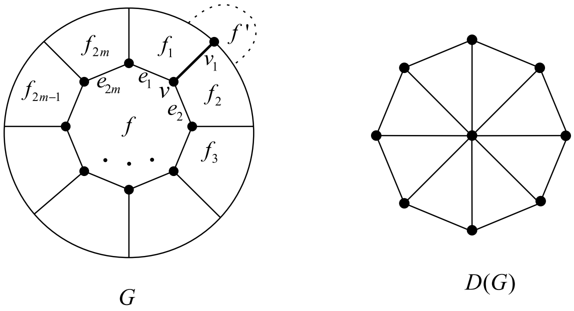

Fig. 3. A 3-resonant polygonal system G and its inner dual $D(G)$.

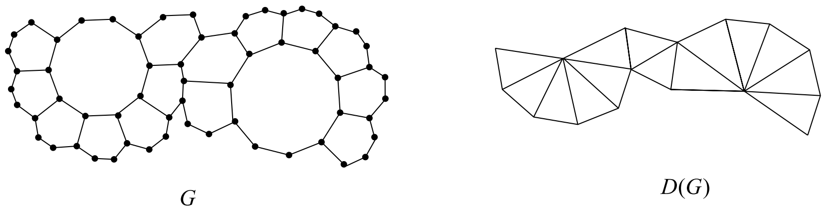

Fig. 4. A 3-resonant polygonal system G and its inner dual $D(G)$.

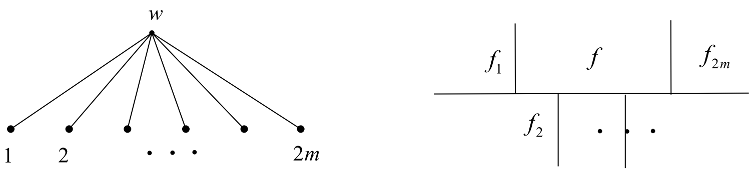

Fig. 5. The illustration for the proof of Lemma 2.6.

A *triangular chain* is a 2-connected outer plane graph consisting of triangles $t_1, t_2, \ldots, t_n$ such that for any i, j with $1 \leqslant i < j \leqslant n$, t_i and t_j share an edge if and only if $j = i + 1$. The length of a path P is the number of edges of P.

Lemma 2.6. *Let G be a 3-resonant polygonal system in $\mathcal{G}$ without separating faces. If G has no internal faces but has inner vertices, then $D(G)$ is a triangular chain with two 2-degree vertices on its ends and each other vertex of odd degree. Moreover, $D(G)$ consists of even triangles.*

Proof. Since G has no internal faces and no separating faces, the inner vertices of G induce a tree T. In fact, T is a path by Lemma 2.4. Note that the triangles of $D(G)$ correspond to the vertices of T one to one. Since T is a path, $D(G)$ is a triangular chain (see Fig. 4).

Each of the first and last triangles of $D(G)$ has a 2-degree vertex, since each of them shares an edge with exactly one other triangle. But each other triangle shares two edges with two triangles. So the other vertices of $D(G)$ have degree more than two.

In fact, we can show that they all have odd degrees. Suppose that a vertex of $D(G)$, say w, has degree $2m$ ($\geqslant 4$). Let f be the face of G corresponding to w and $f_1, f_2, \ldots, f_{2m}$ the neighboring faces of f successively (see Fig. 5). Since G has no internal faces, we may assume that $f_1 \cap f_{2m} = \emptyset$. By Corollary 2.2(b), f_i and f_j are disjoint for $i \neq j \pm 1$. Moreover, G has no separating faces. Hence f_i and f_{i+1} are adjacent for $i = 1, \ldots, 2m-1$. Thus $(\bigcup_{i=1}^{2m} f_i) \cap f$ is a $2m$-length path P. Then $G - f_1 - f_{2m}$ contains an odd component $f - P$. That means that G is not 2-resonant, a contradiction. Hence, all the vertices of $D(G)$ except the two on the ends have odd degrees.

Denote the number of triangles in $D(G)$ by h. Then $|V(D(G))| = h + 2$, where exactly two vertices of $D(G)$ have degree 2 and any other has odd degree. Since the degree sum of any graph is even, h should be even. $\square$

A path P in a graph G is called a *chain* if all internal vertices (not the end vertices) of P have degree 2 but the degree of any end vertex of P is not equal to 2 in G. A chain is even (resp. odd) if it has even (resp. odd) edges. A polygonal system without inner vertices is called *catacondensed*.

Lemma 2.7. *Let G be a 3-resonant catacondensed polygonal system in $\mathcal{G}$. Then $D(G)$ is a tree. Moreover, each chain of G is odd.*

Proof. Since G has no inner vertices, $D(G)$ is a tree. Suppose P is an even chain of G lying on the face f. Suppose that the two ends of P belong to two faces f_1 and f_2 (maybe $f_1 = f_2$) adjacent to f, respectively. Note that in a subgraph formed by three

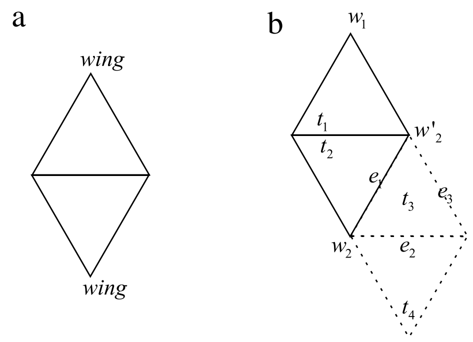

Fig. 6. (a) A kite; (b) The illustration for the proof of Lemma 3.3.

pairwise adjacent faces, there should be inner vertices. Since G is catacondensed, f_1, f_2 may be the same face or disjoint. In either case, $G - f_1 - f_2$ contains an odd component induced by the internal vertices of P. That is a contradiction. □

If a 3-resonant catacondensed polygonal system G has no separating faces, then the cyclomatic number $\gamma(G) \leqslant 2$. The cyclomatic number of a plane graph G is the number of inner faces of G. If $\gamma(G) = 2$, G is the union of two even faces sharing one edge, while if $\gamma(G) = 1$, it is just an even cycle.

3. Construction of 3-resonant polygonal systems in $\mathcal{G}$

We call polygonal systems in $\mathcal{G}$ whose inner dual are described in Lemmas 2.5 and 2.6 *F-type* (flower) and *D-type* (double chain) polygonal systems, respectively. We call those with no even chains, whose inner dual are trees, *T-type* (tree) polygonal systems. In particular, a single even cycle is called the *O-type*. We can see the following.

Proposition 3.1. *There are no* 3*-degree vertices in the subgraph induced by the inner vertices of an F-type, D-type, or O-type polygonal system.*

Still, let $G \in \mathcal{G}$. A subgraph $\mathcal{R}$ of G is called an *even cover* of G if $\mathcal{R}$ is spanning and consists of disjoint faces and odd (length) paths of G, where every vertex of the odd paths is a 2-degree vertex on the boundary of G. Then the following lemma is obvious.

Lemma 3.2. *Let G be a plane graph with an even cover $\mathcal{R}$. Then for any $S \subseteq \mathcal{R}$, both S and $G - S$ have perfect matchings using only edges of $\mathcal{R}$.*

Then we have the following result.

Lemma 3.3. *Let G be a polygonal system of either O-type, F-type, or D-type. Then G has an even cover.*

Proof. O-**type**: G is an even cycle. Then each of its two perfect matchings is an even cover.
F-**type**: Let f be the internal face of G and $f_1, f_2, \ldots, f_{2m}$ be the faces in cyclic order around f. Take out $f_1, f_3, \ldots, f_{2m-1}$. They cover all the vertices of f and themselves. On the other hand, $G - \bigcup_{i=1}^{m} f_{2i-1}$ is a disjoint union of odd paths $P_2, P_4, \ldots, P_{2m}$, where $P_{2i} \subseteq f_{2i}(1 \leqslant i \leqslant m)$ and its every vertex is of 2-degree in G. Then $\{f_1, f_3, \ldots, f_{2m-1}, P_2, P_4, \ldots, P_{2m}\}$ is an even cover of G. In fact, there is another even cover of G, named $\{f_2, f_4, \ldots, f_{2m}, P_1, P_3, \ldots, P_{2m-1}\}$, where P_j is the component of $G - \bigcup_{i=1}^{m} f_{2i}$ on f_j for $j = 1, 3, \ldots, 2m - 1$.
D-**type**: Take $D(G)$ into consideration. Suppose that $D(G)$ has even triangles labeled $t_1, t_2, \ldots, t_{2n}$ successively. Then $t_{2i-1} \cup t_{2i}$ is a kite, named k_i, for each $1 \leqslant i \leqslant n$ (see Fig. 6(a)). $D(G)$ has exactly n kites, any two of which do not share a common triangle. In a single kite k_i, there are two 2-degree vertices which we call wings and two 3-degree vertices adjacent to the wings and lying on both the triangles of k_i.

Let w_1 and w_2 be the two wings of k_1. One of them, say w_2, is a vertex of k_2. We claim that w_2 is also a wing of k_2. If not, w_2 should be a common vertex of t_3, t_4 together with t_2. Suppose that $t_2 \cap t_3 = e_1 = w_2 w_2'$, $t_3 \cap t_4 = e_2$ and e_3 is the third edge of t_3 (see Fig. 6(b)). Then e_3 is a boundary edge, since t_3 is adjacent to at most two triangles. Then w_2' has degree 4. That is impossible as w_2' has odd degree. Hence w_2 is a wing of k_2 and w_2 is not on t_4. Thus w_2 has degree 3.

Then take the second wing of k_2 as w_3 and so on. We can show, by the same argument as above, that w_i is a wing of both k_{i-1} and k_i for $i = 2, 3, \ldots, n$ and has degree 3. At last, take the second wing of k_n (i.e., the other 2-degree vertex of $D(G)$) as w_{n+1}. Let $W = \{w_1, w_2, \ldots, w_{n+1}\}$. Since two wings in a kite are independent and $D(G)$ is an outer plane, W is an independent set. Hence, W corresponds to a disjoint face set R of G.

Let $H = \{h_1, h_2, \ldots, h_t\}$ be all the faces of G corresponding to the non-wing vertices of $D(G)$. For any $h_i \in H$, suppose that h_i corresponds to the non-wing vertex u_i of $D(G)$. Then u_i has odd neighbors inducing a path, say $P = v_1 v_2 \ldots v_{2s-1}$. We claim that $v_1 \in W$. If not, since each triangle of $D(G)$ has one wing, v_2 should be a wing of the kite containing u_i and v_1 as its non-wing vertices. There is an other wing v_2' of this kite adjacent to both u_i and v_1. Since $D(G)$ is an outer plane,

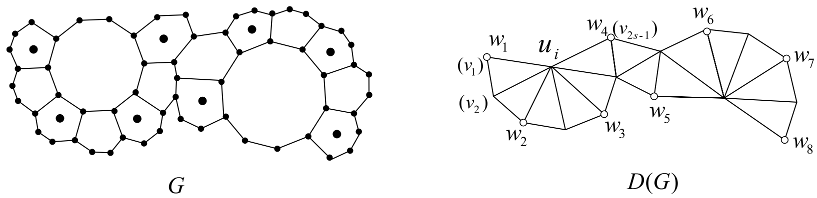

Fig. 7. The faces inscribed within black points in G are the faces of the even cover of G.

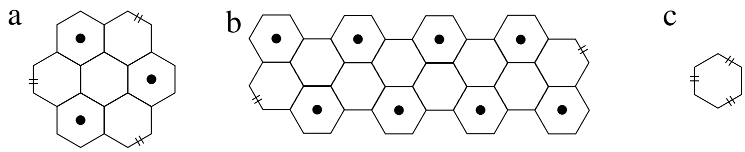

Fig. 8. Examples of the F-type, D-type and O-type polygonal systems together with their even covers: the faces inscribed within black points are the faces in their corresponding even covers and the edges marked are the odd paths.

$v_2' \notin \{v_1, v_2, \ldots, v_{2s-1}\}$. But $v_1, v_2, \ldots, v_{2s-1}$ are all the neighbors of u_i by our assumption, a contradiction. Henceforth, $v_1 \in W$. Successively, $v_{2j-1} \in W$ for each $1 \leqslant j \leqslant s$, since each triangle has exactly one wing (see Fig. 7).

$\{v_1, v_3, \ldots, v_{2s-1}\} \subseteq W$ and thus corresponds to a subset of R. Then $G - R$ contains a component which is an odd path, named P_i, on h_i. Furthermore, vertices of P_i have degree 2 in G. Then $R \cup \{P_1, P_2, \ldots, P_t\}$ is an even cover of G. An example is shown in Fig. 7 and also benzenoid systems with even covers are taken as examples in Fig. 8. $\square$

Let G_1, G_2 be two polygonal systems of either F-type, D-type, or O-type, with even covers $\mathcal{R}_1$ and $\mathcal{R}_2$, respectively. Certainly, each path of $\mathcal{R}_i$ $(i = 1, 2)$ has a perfect matching and we call an edge in this perfect matching an *M-edge* of G_i. Faces of an even cover are called *covering faces* while faces whose boundary contain some path of the even cover are *non-covering*. Note that if G is of F-type or D-type, non-covering faces of G have odd neighboring faces. We define two operations, the gluing operation and the lapping operation, on G_1 and G_2.

Definition 3.4. The gluing operation on G_1 and G_2 along e, denoted by $G_1 \vee_e G_2$, is to patch up G_1 and G_2 by gluing an M-edge of G_1 with one of G_2 into one edge e.

Definition 3.5. The lapping operation on G_1 and G_2 along f, denoted by $G_1 \vee_f G_2$, is to patch up G_1 and G_2 by lapping a non-covering face of G_1 with one of G_2 into one face f such that no vertices of degree more than 3 or even chains are produced.

The common edge and common face of G_1 and G_2 in the two operations are called a *gluing edge* and a *lapping face*, respectively. Fig. 9 gives some examples of the gluing operation and lapping operation.

Let $G_1, G_2, \ldots, G_r$ be a set of polygonal systems of either F-type, D-type, or O-type. Then they have even covers $\mathcal{R}_i$ $(i = 1, 2, \ldots, r)$, respectively. A polygonal system obtained from $G_1, G_2, \ldots, G_r$ by $r-1$ gluing and lapping operations is a graph G obtained from $G_1, G_2, \ldots, G_r$ by running $r-1$ gluing and lapping operations on pairs of them such that G is connected and $G \in \mathcal{G}$. We call G_i $(i = 1, 2, \ldots, r)$ a *segment* of G. Note here, for some face of G, there may be more than one gluing and lapping operation done along it. An example is illustrated in Fig. 10.

Let $G \in \mathcal{G}$. We call a subgraph of G with no separating faces a *non-separating component*, which is called maximal if it is not contained properly in any other one. Let S be a set of vertices of G. An *S-lobe* of G is an induced subgraph of G whose vertex set consists of S and the vertices of a component of $G-S$. For a facial cycle f of G, we use f-lobe shortly for a $V(f)$-lobe.

By Zheng's result [25], each 3-resonant benzenoid system can be obtained from a set of benzenoid systems of the four types in Fig. 1 just by gluing operations. A construction method is presented for all the 3-resonant polygonal systems in $\mathcal{G}$, which contains Zheng's result for benzenoid systems.

Theorem 3.6. *Every* 3*-resonant polygonal system* G *in* $\mathcal{G}$ *can be constructed from* r $(r \geqslant 1)$ F*-type,* D*-type and* O*-type* 3*-resonant graphs by* $r-1$ *gluing and lapping operations on them.*

Proof. Let $G_1, G_2, \ldots, G_t$ be all the maximal non-separating components of G. We shall prove that each of $G_1, G_2, \ldots, G_t$ is of either F-type, D-type, or T-type.

We use induction on t. When $t = 1$, it necessarily holds, since G itself is 3-resonant without separating faces. We suppose that the assertion holds for all integers less than t ($\geqslant$2). Now consider the case t. Choose an arbitrary separating face f of G. Then each f-lobe belongs to $\mathcal{G}$. Next we shall show that each f-lobe is 3-resonant. The following claim is needed.

Claim 1: Let f be any separating face of G. Then chains of G on f are odd, and 3-degree vertices on f induce a union of odd paths.

Proof. Suppose that there is an even chain P on f. Since f is separating, the two ends of P lie on two disjoint faces h_1 and h_2, different from f, in two distinct f-lobes. Hence, $G - h_1 - h_2$ contains an odd component induced by the internal vertices of P. That means G is not 2-resonant, a contradiction. On the other hand, suppose that f has odd 3-degree vertices in some

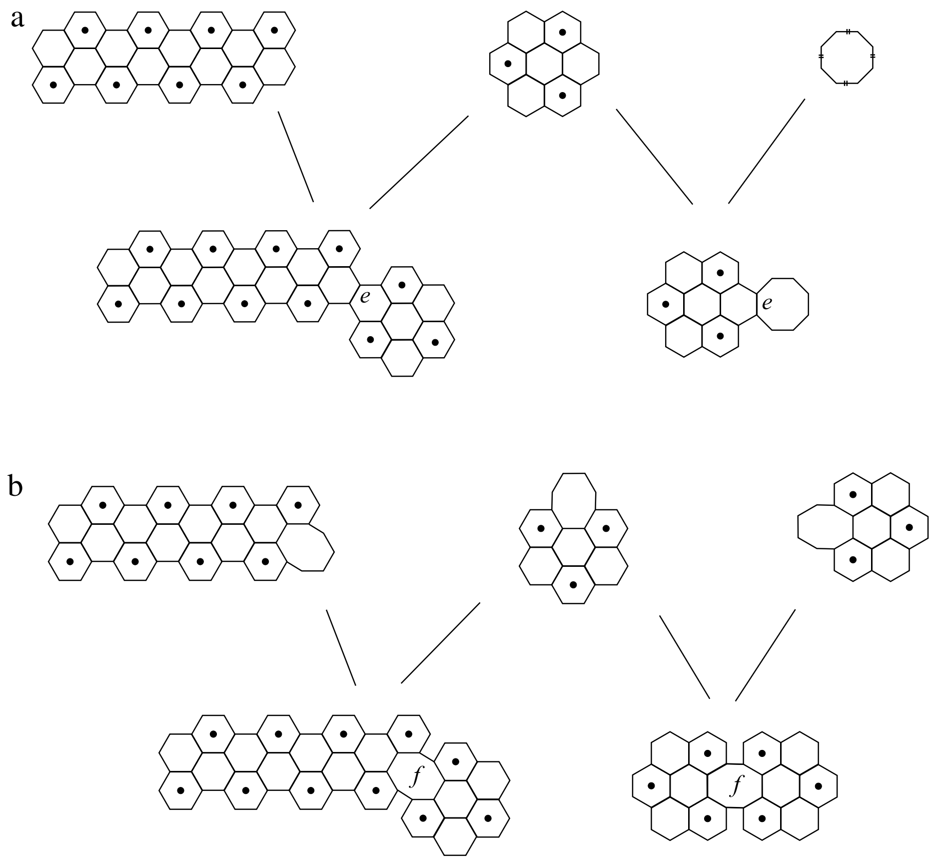

Fig. 9. (a) Examples for the gluing operation; (b) Examples for the lapping operation.

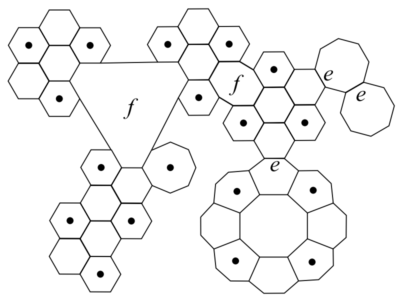

Fig. 10. A 3-resonant polygonal system obtained from 7 F-type, D-type and O-type 3-resonant polygonal systems by 6 gluing operations and lapping operations on them.

f-lobe G'. Let P' be the even path of f induced by these vertices. Then the components of $G' - f$ are components of $G - f$. Since G is 1-resonant, $G' - f$ has even vertices. But then $G - f_1 - f_2$ has odd vertices in this f-lobe, where faces f_1 and f_2 are chosen as shown in Fig. 11. That is also a contradiction. □

Let G' be any f-lobe of G. Then G' must have even vertices. If not, $G - f$ has odd components, which is impossible. Let P be the path of f induced by the 3-degree vertices of f in G' with two ends u and v (see Fig. 12). Then P is an odd path by Claim 1. We assert that G' is 3-resonant. It suffices to show that for any set of no more than three disjoint faces F of G', every component of $G' - F$ has perfect matchings.

Let H be an arbitrary component of $G' - F$. If $f \in F$, then H is also a component of $G - F$. Since G is 3-resonant, H has a perfect matching. Now suppose that $f \notin F$. If $f - P \nsubseteq H$, then H is a component of $G - F$ and thus has a perfect matching. Hence we assume $f - P \subseteq H$. Let M be a perfect matching of $G - F$. If only one of u and v, say u, is matched to its neighbor on $f - P$ in M, then $|V(G') \setminus V(f - (P - u))|$ is even, since these vertices are covered by F or M. But $|V(f - (P - u))|$ is odd. Hence $|V(G')|$ is odd, a contradiction.

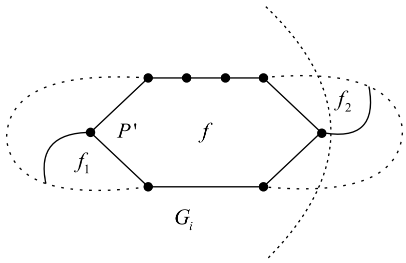

Fig. 11. The illustration for the proof of Claim 1.

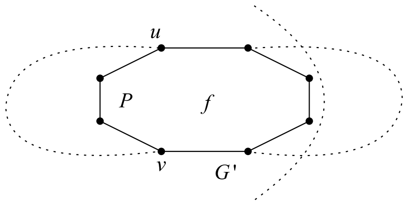

Fig. 12. The illustration for the proof of Theorem 3.6.

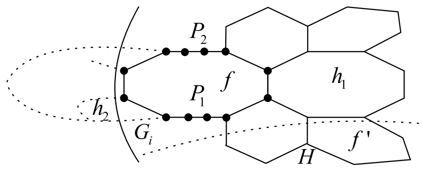

Fig. 13. The illustration for the proof of Claim 2.

Hence, in any perfect matching M of $G - F$, since $|V(G')|$ is even, both u and v match to vertices of $f - P$ or neither do. In both of the cases, H has a perfect matching, which is the union of $M \cap E(H - (f - (P - u - v)))$ and a perfect matching of $f - (P - u - v)$ and the union of $M \cap E(H - (f - P))$ and a perfect matching of $f - P$, respectively. Thus H has a perfect matching. Hence any f-lobe is 3-resonant.

Now we can use induction hypothesis. The maximal non-separating components of each f-lobe are of either F-type, D-type, or T-type by the induction hypothesis. Thus all the maximal non-separating components of all f-lobes, which are exactly $G_1, G_2, \dots, G_t$, are of either F-type, D-type, or T-type.

Note from the above that G is obtained from $G_1, G_2, \dots, G_t$ by lapping common faces (i.e., the separating faces) of pairs of them. To finish the proof of the theorem, we will prove that each of these lapping processes can be viewed as either a gluing operation or a lapping operation. This is immediately obtained following the next several claims.

Claim 2: Let f be a separating face of G. If f is a face of a D-type G_i, then f is non-covering in G_i.

Proof. Suppose to the contrary that f is a covering face of the even cover $\mathcal{R}_i$, obtained in Lemma 3.3, of G_i. Then it corresponds to a wing w of $D(G_i)$ and there is another wing w', which corresponds to face f' in G_i, in the same kite as w. Let h_1 be one of the neighboring faces of f and H the component of $G - f - h_1$ containing $f' - h_1$ (see Fig. 13). Then $V(H)$ is the union of vertices of some components of $G - f - f'$ and $V(f' - h_1)$. Since G is 3-resonant, all the components of $G - f - f'$ are even. Furthermore, $|V(f' - h_1)|$ is even. Hence $|V(H)|$ is even. Moreover, each chain of G on f is odd. Let P_1 be the chain on f with one end adjacent to a vertex of H and h_2 the face containing the other end of P_1 in another f-lobe of G. Denote by H' the component of $G - h_1 - h_2$ that contains H. Then $|V(H')| = |V(H)| + |V(P_1)| - 1$ and thus $|V(H')|$ is odd, a contradiction to the fact that G is 2-resonant. Hence, f cannot be a covering face of G. □

Claim 3: For an F-type G_j, let S be the set of faces of G_j which are separating faces of G. Then either $S \subseteq \{f_1, f_3, \dots, f_{2m-1}\}$ or $S \subseteq \{f_2, f_4, \dots, f_{2m}\}$, where $f_1, f_2, \dots, f_{2m}$ are the faces of G_j in cyclic order around the internal face f' of G_j. Therefore, all the faces in S can be viewed as non-covering faces with respect to one of the two even covers of G_j.

Proof. It suffices to prove that there are no two faces f_i and f_j in S such that i and j have opposite parities. If there are, let f_i and $f_j (i < j)$ be such a pair and further assume that $f_t \notin S$ for any $i < t < j$. Then $G - h_1 - h_2 - f'$ contains an odd component H, where faces h_1 and h_2 are chosen as in Fig. 14, a contradiction. □

Claim 4: The face-lapping process of a T-type G_i and some G_j can be viewed as gluing operations.

Proof. Since the T-type G_i is a maximal non-separating component of G, G_i is a union of two even faces, say f_1 and f_2, sharing an edge named e. Then $G_i = f_1 \vee_e f_2$, where a single even cycle is of O-type. Suppose that G_j is a maximal non-separating

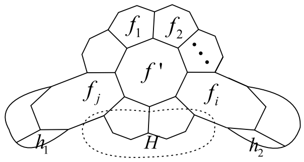

Fig. 14. The illustration for the proof of Claim 4.

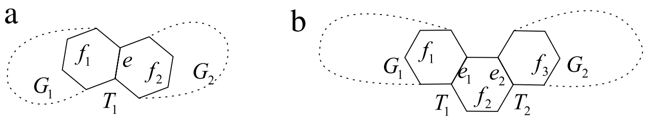

Fig. 15. (a) $G_1 \cup T_1 \cup G_2 = G_1 \vee_e G_2$; (b) $G_1 \cup T_1 \cup T_2 \cup G_2 = G_1 \vee_{e_1} f_2 \vee_{e_2} G_2$, where T_i $(i = 1, 2)$ is the union of f_i and f_{i+1}.

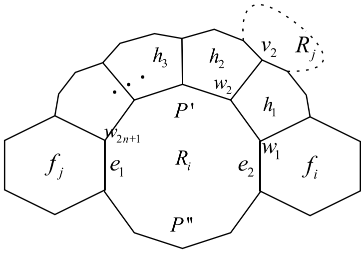

Fig. 16. The illustration for the proof of Lemma 4.1.

component of G that shares f_1 with G_i. If $G_j = f_0 \vee_{e_0} f_1$ for some even face f_0 and edge e_0, then e and e_0 belong to the same perfect matching of f_1 since G has no even chains. Thus $G_j \cup G_i = f_0 \vee_{e_0} f_1 \vee_e f_2$. Otherwise, f_1 is non-covering in G_j by Claims 2 and 3. Since there are no even chains on f_1, e is an M-edge of G_j. Hence, $G_i \cup G_j = f_2 \vee_e G_j$. More examples are shown in Fig. 15. $\square$

By Claims 2 and 3 and the definition of a lapping operation, the face-lapping process of a G_i and a G_j, which are of D-type or F-type, can be viewed as a lapping operation. Together with Claim 4, the proof is finished. $\square$

4. 3-resonant polygonal systems in $\mathcal{G}$ are maximally resonant

We have established a construction method for 3-resonant graphs in $\mathcal{G}$. In this section, we shall show that polygonal systems in $\mathcal{G}$ constructed by our method are maximally resonant. Hence, 3-resonance implies maximal resonance for them.

Lemma 4.1. *Let G be an F-type, D-type, or O-type polygonal system. Then G is k-resonant for any $k \geqslant 3$.*

Proof. If G is of O-type, it is necessarily maximally resonant. We assume that G is of either F-type or D-type. By Lemma 3.3, G has an even cover, say $\mathcal{R}$. It suffices to prove that $G - F$ has a perfect matching for any set F of disjoint faces of G. In fact, we will show a stronger assertion that $G - F$ permits a perfect matching using edges of $\mathcal{R}$ only.

Let $\mathcal{R}' := \{R_i \in \mathcal{R} : R_i \in F$ or R_i is adjacent to some faces of $F\}$. Then $\mathcal{R}' \subseteq \mathcal{R}$ and thus $G - \mathcal{R}'$ has a perfect matching M using only edges of $\mathcal{R}$. If for each $R_i \in (\mathcal{R}' \setminus F)$, $E(F) \cap E(R_i)$ is a subset of a perfect matching of R_i, then the graph $\mathcal{R}' - F$ has a perfect matching, say M'. Thus $M \cup M'$ is a perfect matching of $G - F$ that uses only edges of $\mathcal{R}$ and we are done.

In fact, we shall show that $E(F) \cap E(R_i)$ is indeed a subset of a perfect matching of R_i for each $R_i \in (\mathcal{R}' \setminus F)$. Note that every path of $\mathcal{R}$ belongs to a unique interior face of G. Hence if a path of $\mathcal{R}$ has a common node with F, then the entire path lies on some face of F. Suppose to the contrary that for some face $R_i \in (\mathcal{R}' \setminus F)$, there are $f_i, f_j \in F$ adjacent to R_i and their common edges e_1, e_2 with R_i lie in two different perfect matchings of R_i. Thus $R_i - e_1 - e_2$ consists of two even paths, say P' and P''. Moreover, f_i and f_j are disjoint. Hence the length of each of P' and P'' is at least two. Since R_i is not separating, either all the vertices on P' or all the vertices on P'' are inner vertices of G. Without loss of generality, suppose that all the vertices of P' are inner vertices. Let $P' = w_1 w_2 \ldots w_{2n+1}$ $(n \geqslant 1)$ and $w_r w_{r+1} = h_r \cap R_i$ for $1 \leqslant r \leqslant 2n$ (see Fig. 16). h_r and $h_{r+1}(1 \leqslant r \leqslant 2n)$ have another common vertex, named v_{r+1}, besides w_{r+1}.

Since v_2 is a 3-degree vertex and R_i does not cover it, there is an other $(\mathcal{R} \ni)R_j \neq h_1, h_2$ covering v_2. Then v_2 is an inner vertex. Hence the inner vertex w_2 is adjacent to three inner vertices w_1, w_3 and v_2. That is impossible by Proposition 3.1. Thus $E(F) \cap E(R_i)$ is a subset of a perfect matching of R_i for each $R_i \in (\mathcal{R}' \setminus F)$. $\square$

Note that in the above, an M-edge of G belongs either to $E(F)$ or to perfect matchings of $G - F$ that uses only edges of $\mathcal{R}$.

Lemma 4.2. *Let $G(\in \mathcal{G})$ be a polygonal system obtained from $r(r \geqslant 1)F$-type, D-type or O-type polygonal systems by $r - 1$ gluing and lapping operations on them. Then G is k-resonant for any $k \geqslant 3$.*

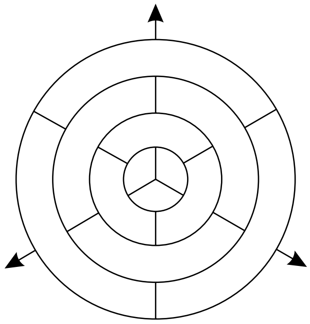

Fig. 17. 3-resonant polygonal systems with faces of size 4.

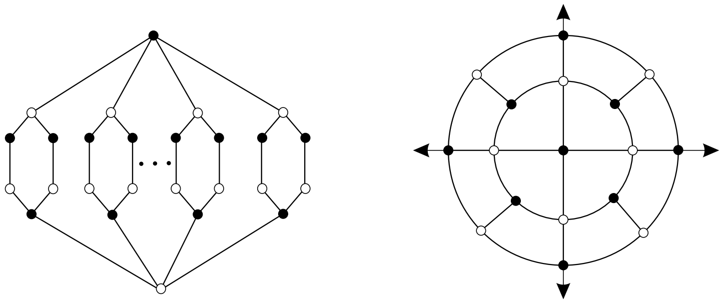

Fig. 18. 3-resonant plane graphs which are not maximally resonant.

Proof. Let $G_1, \ldots, G_r$ be the r F-type, D-type and O-type polygonal systems to form G with even covers $\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_r$, respectively. We shall show a stronger assertion that for any set F of disjoint faces of G, $G - F$ has a perfect matching containing only edges of $\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_r$.

We proceed by induction on r. If $r = 1$, by the proof of Lemma 4.1, $G - F$ has a perfect matching containing only edges of $\mathcal{R}_1$. Suppose the assertion is true for all integers less than r. We consider the case r. Let F be any set of disjoint faces of G. Suppose that G' is the connected subgraph of G that is the union of $G_1, \ldots, G_{r-1}$, and $G = G' \vee G_r$, where $G' \vee G_r$ denotes either a gluing operation or a lapping operation on some G_i $(i \in \{1, 2, \ldots, r-1\})$ and G_r. Let $F_1 = G' \cap F$ and $F_2 = G_r \cap F$.

First suppose that $G' \vee G_r$ is a gluing operation and e is the gluing edge. Then e is an M-edge of both G_i and G_r. Let h_1 and h_2 be the faces of G' and G_r that contain e, respectively. Since F is a disjoint set, at most one of h_1 and h_2 belongs to F. Without loss of generality, suppose that $h_1 \notin F$. By the induction hypothesis, $G' - F_1$ has a perfect matching M_1 containing only edges of $\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_{r-1}$. Then $e \in M_1$. On the other hand, $G_r - F_2$ has a perfect matching M_2 using only edges of $\mathcal{R}_r$. Then $(M_1 - \{e\}) \cup M_2$ is the desired perfect matching of $G - F$.

Otherwise, suppose that $G' \vee G_r$ is a lapping operation and f is the lapping face. Let $P_1, \ldots, P_t$ be the paths of f induced by 3-degree vertices of f in G' and P_r the one in G_r. Then these paths are all odd paths, since every lapping face has odd neighboring faces in an F-type or D-type segment of $\mathcal{G}$.

Case 1: $f \in F$.

By the induction hypothesis, both $G' - F_1$ and $G_r - F_2$ have perfect matchings, say M_1 and M_2, respectively, using only edges of $\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_r$. Then $M_1 \cup M_2$ is the desired perfect matching of $G - F$.

Case 2: $f \notin F$.

Since f is a lapping face, it is non-covering in any segment of G containing it and there are no even chains of G on f. By the induction hypothesis, $G' - F_1$ has a perfect matching M_1 containing only edges of $\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_{r-1}$, which restricted on P_r and chains of G on f are perfect matchings of them. Symmetrically, $G_r - F_2$ has a perfect matching M_2 using only edges of $\mathcal{R}_r$, which restricted on $P_1, \ldots, P_t$ and chains of G on f are perfect matchings of them. Then $(M_1 - E(P_r)) \cup (M_2 - E(\bigcup_{i=1,\ldots,t} P_i))$ is the desired perfect matching of $G - F$. $\square$

Theorem 3.6, Lemmas 4.1 and 4.2 yield the main results of this paper.

Theorem 4.3. *A polygonal system in $\mathcal{G}$ is k-resonant ($k \geqslant 3$) if and only if it can be obtained from $r(r \geqslant 1)$F-type, D-type or O-type polygonal systems by $r - 1$ gluing and lapping operations on them.*

Theorem 4.4. *Let $G \in \mathcal{G}$. Then G is maximally resonant if and only if it is 3-resonant.*

Corollary 4.5 ([24]). *A 3-resonant benzenoid system is maximally resonant.*

Corollary 4.6. *All 3-resonant catacondensed polygonal systems in $\mathcal{G}$ are maximally resonant.*

It can be seen that Lemma 2.7 and Corollary 4.6 still hold if those catacondensed polygonal systems contain faces of size 4. In fact, if faces of size 4 exist, then the characterizations of Lemma 2.6 are still valid and the equivalent relation between 3-resonance and maximal resonance also holds.

However, for polygonal systems with internal faces, Lemma 2.5 does not always hold in the case when faces with size 4 occur. See the graph in Fig. 17 for instance. The maximal resonance of polygonal systems with faces of size 4 remains open.

On the other hand, a 3-resonant plane bipartite graph is not necessarily maximally resonant. There are two examples in Fig. 18.

Acknowledgements

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References

[1] R. Chen, X. Guo, *k*-coverable coronoid systems, J. Math. Chem. 12 (1993) 147–162.
[2] E. Clar, The Aromatic Sextet, Wiley, London, 1972.
[3] X. Guo, *k*-resonance in benzenoid systems, open-ended carbon nanotubes, toroidal polyhexes; and *k*-cycle resonant graphs, MATCH Commun. Math. Comput. Chem. 56 (2006) 439–456.
[4] D.J. Klein, Elemental benzenoids, J. Chem. Inf. Comput. Sci. 34 (1994) 453–459.
[5] Q. Li, S. Liu, H. Zhang, 2-extendability and *k*-resonance of non-bipartite Klein-bottle polyhexes, preprint, 2009.
[6] K. Lin, R. Chen, *k*-coverable polyhex graphs, Ars Combin. 43 (1996) 33–48.
[7] M. Randić, Conjugated circuits and resonance energies of benzenoid hydrocarbons, Chem. Phys. Lett. 38 (1976) 68–70.
[8] M. Randić, On the characterization of local aromatic properties in benzenoid hydrocarbons, Tetrahedron 30 (14) (1974) 2067–2074.
[9] M. Randić, Graph theoretical approach to local and overall aromaticity of benzenoid hydrocarbons, Tetrahedron 31 (11–12) (1975) 1477–1481.
[10] M. Randić, Aromaticity and conjugation, J. Amer. Chem. Soc. 99 (1977) 444–450.
[11] M. Randić, Conjugated circuits and resonance energies of benzenoid hydrocarbons, Chem. Phys. Lett. 38 (1976) 68–70.
[12] M. Randić, Aromaticity of polycyclic conjugated hydrocarbons, Chem. Rev. 103 (9) (2003) 3449–3605.
[13] W.C. Shiu, P.C.B. Lam, H. Zhang, *k*-resonance in toroidal polyhexes, J. Math. Chem. 38 (4) (2005) 451–466.
[14] W.C. Shiu, H. Zhang, A complete charaterization for *k*-resonant Klein-bottle polyhexes, J. Math. Chem. 43 (2008) 45–59.
[15] W.C. Shiu, H. Zhang, S. Liu, Maximal resonance of cubic bipartite polyhedral graphs, J. Math. Chem., in press (doi:10.1007/s10910-010-9700-8). Published online 12 June 2010.
[16] D. Ye, Z. Qi, H. Zhang, On *k*-resonant fullerene graphs, SIAM J. Discrete Math. 23 (2) (2009) 1023–1044.
[17] F. Zhang, R. Chen, When each hexagon of a hexagonal system covers it, Discrete Appl. Math. 30 (1991) 63–75.
[18] F. Zhang, L. Wang, *k*-resonance of open-ended carbon nanotubes, J. Math. Chem. 35 (2) (2004) 87–103.
[19] F. Zhang, M. Zheng, Generalized hexagonal systems with each hexagon being resonant, Discrete Appl. Math. 36 (1992) 67–73.
[20] H. Zhang, S. Liu, 2-resonance of plane bipartite graphs and its applications to boron–nitrogen fullerenes, Discrete Appl. Math. 158 (2010) 1559–1569.
[21] H. Zhang, D. Ye, On *k*-resonant toroidal polyhexes, J. Math. Chem. 44 (2008) 270–285.
[22] H. Zhang, F. Zhang, Plane elementary bipartite graphs, Discrete Appl. Math. 105 (2000) 291–311.
[23] H. Zhang, F. Zhang, Perfect matchings in polyomono graphs, Graphs and Combin. 13 (1997) 295–304.
[24] M. Zheng, *k*-resonant benzenoid systems, J. Mol. Struct. (Theochem) 231 (1991) 321–334.
[25] M. Zheng, Construction of 3-resonant benzenoid systems, J. Mol. Struct. (Theochem) 277 (1992) 1–14.